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Prof. Geoffrey M. Lilley to Join ICASE

Professor Geoffrey M. Lilley, a world renowned fluid dynamicist and an expert on turbulence and acoustics, will join ICASE in April 1998 as Chief Scientist for Fluid Mechanics. In this position, Prof. Lilley will have considerable independence to expand ICASE's aeroacoustics program through interactions, collaborations, and mentorship of ICASE staff scientists, ICASE consultants, as well as NASA and industry research scientists.

Prof. Lilley obtained the B.Sc. degree in Engineering with First Class Honors from Imperial College in 1943. Later, in 1945, under the supervision of Professors Sir Leonard Bairstow and Sir George Temple, Prof. Lilley obtained the M. Sc. and D.I.C. degrees also from Imperial College.

In October 1946, the College of Aeronautics at Cranfield was established in an airfield used by the RAF. The training at Cranfield was to be at the post graduate level with research to be undertaken by staff and students. Prof. Lilley joined the College as a founding member and lectured until 1955. In 1955, he was appointed Deputy Head of the College of Aeronautics. Prof. Lilley held this position for 8 years until he joined the University of Southampton as Professor and Head of the Aeronautics and Astronautics Department in 1963. He remained Department Head for 15 years. In 1983, Prof. Lilley became Professor Emeritus.

Prof. Lilley's long career has provided him with a wealth of knowledge and experience in both theoretical and experimental aspects of fluid mechanics. He has been responsible for the design, manufacture, and installation of many wind tunnels at Cranfield. He has also published and made im-

portant contributions in the fields of aeroacoustics, flutter, sonic boom, turbulence, aerodynamics of road vehicles, human-powered flight, theory of jets, propeller-wing interference, and the design of supersonic civil transport and AVSTOL aircraft.

Among the many honors he has received, particularly worth mentioning are the Gold Medal of the Royal Aeronautical Society in 1983 and the AIAA Aeroacoustic Medal in 1984.



Professor Geoffrey Lilley

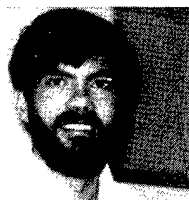
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ICASE: In Retrospect



Amiram "Ami" Harten
9/22/46-8/5/94
Visiting Scientist,
Consultant ('76-'94)



David Kamowitz
10/15/58-9/16/89
Staff Scientist ('86-'89)



Milton E. "Milt" Rose
5/22/25-8/22/93
Director ('77-'86)

Message from the Director, Manuel D. Salas

The success ICASE has had over the last 25 years in advancing research in applied mathematics, computer science, and fluid mechanics has been a result of the vision of its former directors, the excellence of its scientific staff and consultants, and the dedication and commitment of its administrative staff. We dedicate this issue of the quarterly to the memory of Ami Harten, David Kamowitz, and Milt Rose. They are greatly missed by their friends and colleagues; their contributions to science live on.

Ami Harten was a brilliant scientist. He pursued his doctoral studies under Peter Lax at the Courant Institute of Mathematical Sciences. His short career was extremely influential to those involved in the numerical solution of hyperbolic conservation laws. Among his many contributions are his work on Total-Variation-Diminishing schemes and Essentially Non-Oscillatory schemes. Ami was a cheerful, outgoing fellow, always willing to share his insights and engage in friendly discussion. His visits to ICASE for a period covering 18 years always enriched the atmosphere of the institute.

David Kamowitz came to ICASE in 1986. His Ph.D. work, under Seymour Parter at the University of Wisconsin, was on multigrid methods for elliptic boundary value problems. He was diagnosed with a rare form of cancer in the spring of 1987. Throughout his two and a half year ordeal, he was incredibly optimistic and courageous. Despite his illness, he made contributions to the numerical implementation of outflow boundary conditions and the application of multigrid to singular perturbation problems.

Milton E. Rose had probably the greatest influence in setting ICASE's future course. I met him when he became ICASE Director in 1977. Milt, as he liked to be called, was a career administrator with a love for mathematics and a sharp sense for identifying young, talented scientists. His doctoral advisor, Richard Courant, taught him the importance of understanding and incorporating physical ideas into computational mathematics. His interest in computational fluid dynamics, his gentle, modest nature, and his disdain for bureaucracy was an instant hit with me and we remained close friends until his death in 1993. Hanging on my wall is a letter he wrote to me on April 8, 1981. His enthusiasm for carrying out research and his humble nature rings through it. His signature now fading, it reads:

Dear Manny:

Our experiments have been sidetracked. . . Simply stated, these arose from an unsuccessful attempt to impose dissipative boundary conditions at all boundaries. . .

. . . I am focusing upon treating some simpler problems. . . Hopefully, with these clarified, a more focused attempt to understand the remaining problems can be undertaken.

Friedrichs once complained to me that applied mathematicians (he included) seem to engage themselves in clarifying methods which scientists and engineers have already established! I'm reminded of the story of the fellow who enjoyed show business - his job was sweeping the excrement [Milt used a shorter, more descriptive word] of the elephants in the circus! Sometimes I think of this when I attempt to catch up to where. . . others are (and have already passed!).

Well, we also serve who only sweep!

Milt.

ICASE Administrative Staff



Front row, l-to-r: Gwendolyn W. Wesson - Contract Accounting Clerk (1994); Linda T. Johnson - Office and Financial Administrator (1974)

Back row: Barbara A. Cardasis - Administrative Secretary (1986); R. Anne Lomas - Payroll and Accounting Clerk (1992); Etta M. Blair - Accounting Supervisor (1984); Emily N. Todd - Conference Manager (1982); Shelly M. Johnson - Executive Secretary/Visitor Coordinator (1989)

Current ICASE Staff

(ANM = Applied and Numerical Mathematics; CS = Computer Science; FM = Fluid Mechanics)

Research Fellows:

| | |
|--------------------|-------|
| Mavriplis, Dimitri | (ANM) |
| Mehrotra, Piyush | (CS) |

Associate Research Fellow:

| | |
|-----------------|------------|
| Keyes, David E. | (CS & ANM) |
|-----------------|------------|

Senior Staff Scientists:

| | |
|----------------------|-------|
| Crockett, Thomas W. | (CS) |
| Girimaji, Sharath S. | (FM) |
| Lewis, R. Michael | (ANM) |
| Lončarić, Josip | (ANM) |
| Ristorcelli, J. Ray | (FM) |
| Sidilkover, David | (ANM) |
| Zhou, Ye | (FM) |

Staff Scientists:

| | |
|-------------------------|-------|
| Allan, Brian G. | (ANM) |
| Arian, Eyal | (ANM) |
| Guattery, Stephen M. | (CS) |
| Interrante, Victoria L. | (CS) |
| Luo, Li-Shi | (FM) |
| Ma, Kwan-Liu | (CS) |
| Povitsky, Alexander | (FM) |

System Administrators:

| |
|-----------------|
| Clancy, Leon M. |
| Hess, Bryan K. |

ICASE currently has 14 graduate students and three visiting scientists.

ICASE Directors

| | |
|-----------------------------|--------------|
| James M. Ortega | 1972-1977 |
| Milton E. Rose | 1977-1986 |
| Robert G. Voigt | 1986-1991 |
| M. Yousuff Hussaini | 1992-1996 |
| (Acting Director 1991-1992) | |
| Manuel D. Salas | 1996-present |

Facts About ICASE

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| ICASE Technical Reports to Date | 1,440 |
| Conferences/Workshops/Short Courses | 55 |
| Hardbound Volumes Published (since 1992) | 20 |

3D Flow Visualization Using Volume Line Integral Convolution

Victoria Interrante¹ and Chester Grosch²

Introduction

Line integral convolution (LIC) is a flow-driven texture generation method that has become one of the best-known and most commonly used techniques in computer graphics for visualizing 2D flow, or flow over a surface in 3D. The popularity of LIC as a tool for 3D flow visualization, or the depiction of flow through a volume, has been relatively limited in contrast, however, primarily due to the difficulties inherent in clearly and effectively portraying a dense volume texture in a static, 2D image. Over the past months, we have been investigating strategies for more effectively using 3D LIC for the visualization of 3D flow. Much of this work is described in our ICASE Report No. 97-35. In this article we highlight new results from our continuing work in this area.

Background and Motivation

Given a vector field and an input texture, line integral convolution produces an output texture in which the data values are highly correlated in the direction of the flow. Our work focuses on methods for effectively representing the flow information contained in the dense volumetric textures produced by 3D LIC. Our strategies include selectively emphasizing flow information in critical regions of interest in the volume and clarifying the 3D structure of the flow by facilitating the perceptual differentiation of the densely clustered streamlines.

Region of Interest Definition

By concentrating the 3D texture in the most significant areas of the flow, we can clarify the visual representation of the data and facilitate the appreciation of the most relevant information.

When LIC is used in conjunction with a region of interest (ROI) definition based on the value of a scalar quantity across the volume, we have found that best results are achieved when the ROI mask is applied to the *input* texture rather than to the output. Figure 1 compares the two effects.

¹Dr. Interrante received her Ph.D. from the University of North Carolina at Chapel Hill, and joined ICASE as a Staff Scientist in 1996.

²Dr. Grosch is a Professor of Oceanography and Computer Science at Old Dominion University. He has been a consultant at ICASE since 1980.

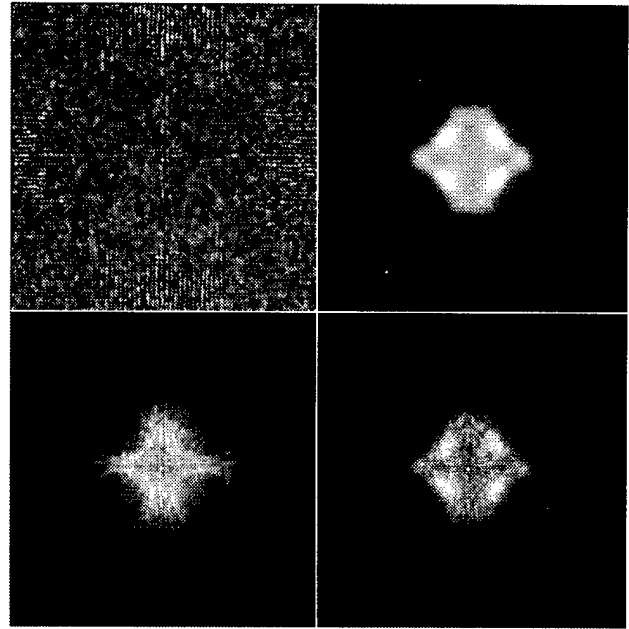


Figure 1: Clockwise from upper left: a 2D slice from a 3D LIC texture; a region of interest mask, defined by velocity magnitude; results when the ROI mask is applied to the texture generated by LIC; results when the ROI mask is applied, as a preprocess, to the input texture whose values are then convolved by LIC.

When the ROI mask is applied as a post process, the visibility of the flow information is directly defined by the values in the ROI, whose edges are not, in general, guaranteed to be everywhere tangent to the direction of the flow. When the ROI mask is applied as a preprocess, the same basic segmenta-

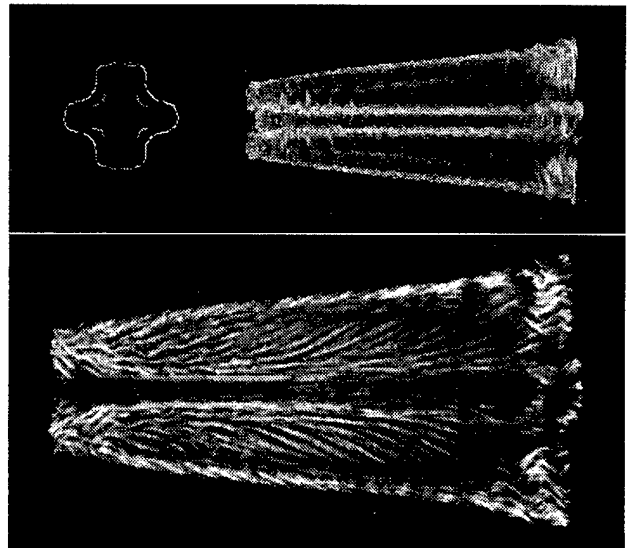


Figure 2: Upper: ridges of velocity magnitude can be used to define a surface of interest in the flow; Lower: 3D LIC applied to a texture of points evenly distributed over this velocity ridge surface.

tion is in effect, however the flow itself is allowed to define the explicit boundaries of the visible information.

Figure 2 illustrates a second method for ROI definition. Here, a ridge-finding algorithm is used to define a precise *surface* of interest in the volume, and the LIC texture is derived from a set of Gaussian spots uniformly distributed over this surface. However, the directional information is not projected onto the 2D surface. All calculations are done in 3D, so that the tufts in the output texture will accurately reflect the local 3D orientation of the flow in the immediate vicinity of the specified surface of interest.

Clarifying the Dense Texture Data

When the LIC output densely occupies a 3D region of space, individual streamlines can be difficult to discriminate due to their similar shading. The three-dimensional spatial relationships among the overlapping streamlines represented in the LIC texture volume will be clarified if the depth discontinuities in the scene are emphasized through the use of 'visibility-impeding halos', as demonstrated in Figure 3.

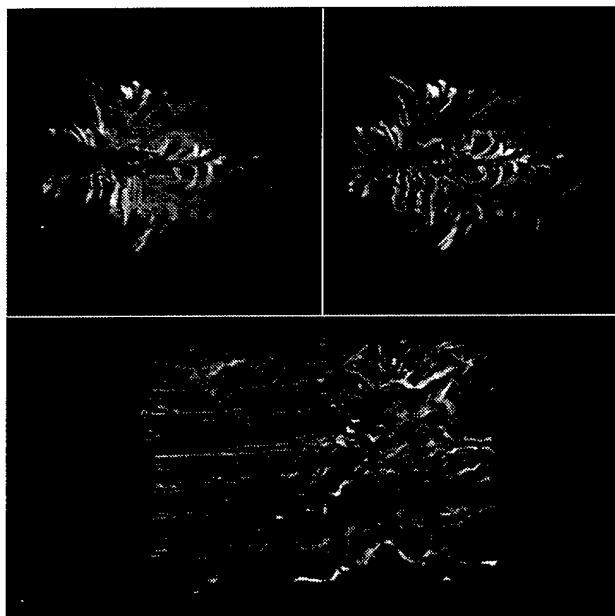


Figure 3: Upper left: volume rendered streamlines in a flow through a circular jet with tabs; Upper right: visibility-impeding halos emphasize depth discontinuities; Bottom: haloed streamlines in a flow through a rectangular aperture.

Information about the forward/backward direction of the flow can be incorporated into a static 2D image through the use of tapered streamlines.

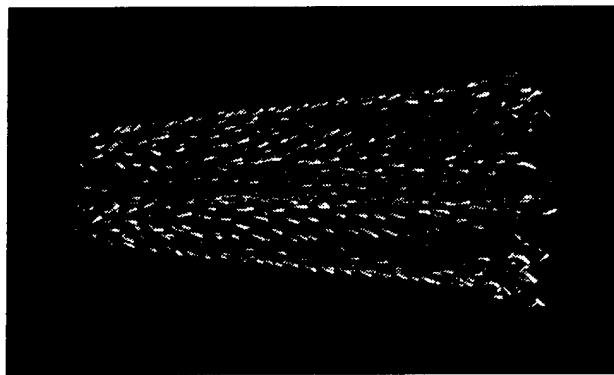


Figure 4: Tapered streamlines convey the forward/backward direction of the flow.

A simple modification to the fast-LIC algorithm allows the efficient computation of oriented streamlines, as shown in Figure 4. This modification is based on the use of an asymmetric filter of the form:

$$I'_0 = \sum_{i=0}^{flength} v_i c^i, \quad c < 1$$

in place of a simple box filter. Texture values at subsequent voxels along a streamline may still be computed incrementally based on previous values:

$$I'_1 = (I'_0 - v_0)/c + v_{flength+1} c^{flength}$$

$$I'_{-1} = (I'_0 - v_{flength} c^{flength})/c + v_{-1}.$$

Future Work

We are continuing to investigate methods for more efficiently generating smooth, cyclic animations of 3D LIC textures along streamlines in steady flow data, and are actively working on extending our 3D LIC algorithm to the visualization of streaklines in 3D unsteady flow data.

References

- V. Interrante and C. Grosch, "Strategies for Effectively Visualizing 3D Flow with Volume LIC," *Proceedings of IEEE Visualization '97*, pp. 421 - 424.
- C. E. Grosch, J. M. Seiner, M. Y. Hussaini and T. L. Jackson, "Numerical Simulation of Mixing Enhancement in a Hot Supersonic Jet," *Physics of Fluids*, 9(4): 1125 - 1143, 1997.
- V. Interrante, "Illustrating Surface Shape in Volume Data via Principal Direction-Driven 3D Line Integral Convolution," *Computer Graphics Proceedings, Annual Conference Series*, pp. 109 - 116.

Eigenvalue Bounds Using Graph Embeddings

Stephen Guattery¹

Introduction and Motivation

Combinatorial techniques provide a useful way of bounding extreme eigenvalues of Laplacian and related matrices. Any symmetric matrix can be described in terms of a weighted underlying graph. To construct bounds, one first constructs embeddings of pairs of these graphs into each other, then derives quantities that characterize the embedding. Bounds are computed from these quantities. Embedding methods have the advantage that they can often be applied to classes of matrices: specifying the form of the embedding for the class yields bounds for all members of the class. While these techniques were originally developed for Laplacian matrices, a number of recent developments have extended them to more general classes of symmetric, positive definite matrices. We review some bounding techniques and discuss how they have been extended.

Bounds on the extreme eigenvalues have many uses. The Laplacian is used in representing physical problems involving elliptic partial differential equations. Since these matrices are symmetric, their extreme eigenvalues can be used in computing their spectral condition numbers, which are used to bound the rates of convergence of iterative linear system solvers, and to analyze the quality of preconditioners.

The smallest nonzero eigenvalue λ_2 of a Laplacian is related to properties of the associated graph. This connection has been exploited in the design and analysis of graph algorithms, particularly algorithms for finding small separators: Bounds on λ_2 can be used to compute bounds on cut quality and to isolate the structure of the eigenvectors on which the cuts are based. The eigenvalue λ_2 is also related to expansion properties of graphs, and can be used to determine if a graph is an expander.

Laplacians, Graphs, and Embeddings

A Laplacian matrix can be defined in terms of a graph as follows: Let G be an undirected graph with vertices v_1, \dots, v_n . Then the *Laplacian* of G

is an $n \times n$ matrix L such that

$$l_{ij} = \begin{cases} \text{degree}(v_i) & \text{if } i = j \\ -1 & \text{if } (i, j) \text{ is an edge of } G \\ 0 & \text{otherwise.} \end{cases}$$

Laplacians are symmetric and have all row sums equal to zero. We assume for the discussion below that the matrix is irreducible, which corresponds to assuming that G is connected.

The definition can be extended to weighted graphs if the nonzero off-diagonal entries have negative values other than -1 ; these entries are the negatives of the weights of the edges in the graph. In this case we define the degree of a vertex to be the sum of the weights of its incident edges. In either the unweighted or weighted case, if the row sums are not equal to zero, we can think of the surplus (or deficiency) of the sum for row i as representing the weight of an edge to a zero Dirichlet boundary, which can be represented as a single ground vertex in the graph. This vertex is implicit in the matrix structure.

The techniques discussed below make use of graph embeddings: Let G and H be connected graphs on the same set of vertices. An *embedding* of G into H is a set of paths in H such that for every edge (i, j) in G , the set includes a path from vertex i to vertex j .

Note that an edge in H could end up on more than one path. To capture this possibility, we introduce the idea of *congestion*. Congestion is simple in the unweighted case: the congestion of an edge e in H is the number of paths in the embedding that include e . In the weighted case, we assign each path the weight of the corresponding edge in G . The congestion of an edge e in H is the sum of the weights of the paths that include e divided by the weight of e . The congestion of a path is the sum of the congestions of the edges in the path.

The Path Resistance Method

Using the ideas of graph embeddings and path resistances, Guattery, Leighton, and Miller have shown a way to compute a lower bound on the smallest nonzero eigenvalue λ_2 of a Laplacian. Let G be the underlying graph of the Laplacian L ; for simplicity, we assume that G is unweighted. Let K be the complete graph on the n vertices of G (a complete graph has an edge between every pair of vertices). The bound is based on an embedding of

¹Dr. Guattery received his Ph.D. from Carnegie Mellon University. He joined ICASE as a Staff Scientist in 1995.

K into G . The technique is called the *path resistance method*, and is described as follows:

1. Construct a path embedding of K into G .
2. Compute the congestion c_{ij} of each edge (i, j) in G .
3. For each path P , allocate a resistor of size c_{ij} to edge e_{ij} on P .
4. For each path P compute its resistance as a series resistive circuit, i.e., $\sum_{e_{ij} \in P} c_{ij}$. Let r be the maximum resistance over all paths.
5. return " $n/r \leq \lambda_2$ ".

The proof that this procedure gives a lower bound is based on decomposing the problem into edges from K and corresponding paths in G . Each edge in each path in G is scaled by its congestion. The resulting path problems have an interpretation in terms of the theory of resistive circuits, hence the name "path resistance method."

The path resistance method can be extended in a number of ways. Some of the extensions allow its application to a wider range of graphs including weighted graphs and diagonally dominant graphs with positive off-diagonal entries. Another extension lets the method be used with Laplacians with zero Dirichlet boundary conditions; this variant embeds a star rather than a complete graph. Finally, priorities can be assigned to paths in the embedding; these priorities affect the relative amounts of congestion produced by various paths, and can be used in certain cases to give better lower bounds.

The best bounds produced by the path resistance method using priorities are not tight. This is a consequence of a result by Nabil Kahale. However, Guattery, Leighton, and Miller have shown that for the Laplacian of any unweighted tree T , the path resistance method as stated above (i.e., using uniform priorities) gives a lower bound that is off by at most a factor of $O(\log \text{diameter}(T))$.

Embeddings, Generalized Eigenvalues, and Spectral Condition Numbers

In his Ph.D. thesis, Keith Gremban used similar techniques for bounding spectral condition numbers of preconditioned systems. In particular, if A and B are positive definite Laplacians, he has shown how to use embedding techniques to give an

upper bound on $\kappa(B^{-1}A)$, where κ is the spectral condition number. Gremban's techniques require embedding B into A and A into B .

Gremban used the results to bound the condition number of Support Tree Preconditioners, which are tree-structured preconditioners built on an extended vertex set (i.e., the matrix for the preconditioner has a somewhat larger order than the original matrix). Because of the tree structure, these preconditioners are amenable to fast parallel computation in preconditioned conjugate gradient calculations.

Gremban gives extensions to cases where A and B may have positive off-diagonal entries, but requires that the matrices be diagonally dominant. Guattery has given an extension to non-diagonally dominant positive definite matrices, which allows for incomplete factor preconditioners.

We have successfully applied these techniques to a wide variety of preconditioners including Support Tree preconditioners, preconditioners based on incomplete Cholesky factorization, block diagonal domain decomposition preconditioners, and preconditioners for various basic iterative methods.

An Exact Relationship Between Embeddings and Eigenvalues

As noted above, the bounds produced by these embedding methods are not tight. However, there is a fundamental connection between embeddings and graph spectra. Guattery and Miller have shown that, by changing the representation of the embedding to include (arbitrary) edge directions, it is possible to use a specific embedding to produce a matrix whose eigenvalues have a reciprocal relationship to those of the original matrix. For nonsingular symmetric matrices, this technique can be used to find their inverses. We are looking into practical applications of this development.

References

- S. Guattery, T. Leighton, and G. L. Miller "The Path Resistance Method for Bounding the Smallest Nontrivial Eigenvalue of a Laplacian," *ICASE Technical Report 97-51*.
- S. Guattery, "Graph Embedding Techniques for Bounding Condition Numbers of Incomplete Factor Preconditioners," *ICASE Technical Report 97-47*.
- S. Guattery and G. L. Miller "Graph Embeddings and Laplacian Eigenvalues," *ICASE Technical Report*, in preparation.

CACHE-EFFICIENT ALGORITHMS FOR IRREGULAR COMPUTATIONS

Alex Pothen¹

Introduction and Motivation

Consider a computation on an unstructured mesh, where the values at a mesh point are updated using the current values at the neighbors of that mesh point. Examples of such computations abound in scientific computing. In what order should we visit the mesh points to compute the value at each point so that the computation is as fast as possible?

Observe that the arithmetic operations (typically in floating point for scientific computations) are the same for different orders in which we visit the mesh points. Nevertheless, on modern superscalar workstation architectures, one ordering might perform an order of magnitude faster than another ordering. The reason is that the performance of an algorithm on these architectures is limited by how fast the memory can satisfy the voracious appetite of the CPU for data. A fast and small memory called the cache is used to feed the CPU quickly with the data that it needs to compute. When the CPU finds the data it needs in the cache, then the computations proceed without delay; when the data is not in the cache, then several cycles need to be spent fetching the data from the primary memory into the cache. As modern microprocessor architectures seek to boost performance by enhancing the number of instructions that can be executed in parallel with pipelining, replicated functional units, branch prediction, and multiple issue, it is crucial to ensure that the algorithm performs the irregular computation in an order that keeps the number of cache misses as small as possible.

Choosing a cache-efficient ordering for an unstructured mesh or irregular graph is no simple matter. In recent work with Dr. Horst Simon, Professor Alan George, Dr. Steve Barnard, and Gary Kumfert, we have described two ordering algorithms for “inducing locality” in irregular meshes or graphs, and thereby reduce the number of cache misses. One of these algorithms is combinatorial in nature, and is related to algorithms that were

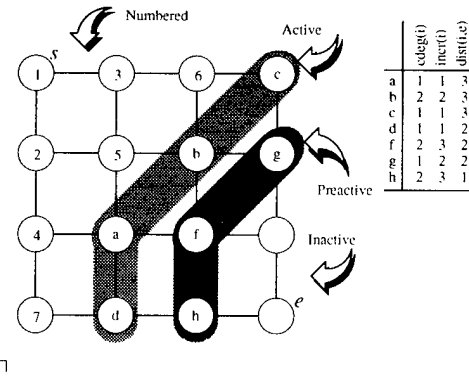


Figure 1: A snapshot of the Sloan algorithm in progress.

proposed earlier for this problem. The second is an algebraic algorithm, and is currently the algorithm that computes orderings of the best quality for this problem. Its somewhat intriguing success can be justified by formulating a simplified problem as a quadratic assignment problem (a combinatorial optimization problem). The rest of this article will describe these results in more detail.

Wavefront Minimization

The problem considered at the beginning of this article can be formulated as a problem called the wavefront minimization problem. At any stage in the computation, the i th wavefront is the number of unvisited mesh points that are neighbors of the i mesh points that have been visited. We seek to minimize the sum of all the wavefronts as the number of mesh points visited ranges from one to the total number of mesh points.

The wavefront minimization problem has been studied in the sparse matrix algorithms community because of its applications in frontal solvers used in structural analysis, and in incomplete factorization preconditioners.

The Sloan Algorithm

A combinatorial algorithm due to Sloan, an Australian civil engineer, and developed further by Iain Duff, John Reid, and Jennifer Scott at the Rutherford Appleton Laboratory in Oxford, is currently the best in its class in terms of computing the lowest values of the total wavefront. This algorithm takes a *yin and yang* approach to the wavefront problem, balancing the conflicting needs of taking a global viewpoint of the mesh while locally controlling the increase in wavefront as it chooses the next meshpoint to be visited.

Sloan’s algorithm is a graph traversal algorithm

¹Dr. Pothen is an Associate Professor in the Computer Science Department at Old Dominion University, Norfolk, VA. He has been a consultant at ICASE since 1994.

that has two parts. The first part selects a start vertex s and an end vertex e that are about as far apart from each other in the mesh as possible. This is done by a few breadth-first-searches in the mesh. The second part then numbers the vertices, beginning from s , choosing the next vertex to number from a set of eligible vertices by means of a priority function. Roughly, the priority of a vertex has a local and global component: the local component favors a vertex that increases the current wavefront the least, while the global part favors vertices at the greatest distance from the end vertex e .

The figure shows a snapshot of the Sloan algorithm. Seven vertices have been ordered, and the vertices eligible to be numbered next are neighbors of the ordered vertices, or their neighbors (the shaded vertices). From among these vertices, a vertex of largest priority is chosen.

Our improvements to the Sloan algorithm

Last year, Gary Kumfert and I provided an implementation of this algorithm whose running time is bounded in the number of edges in the mesh; earlier implementations had time requirements that were nonlinear in the size of the problem, $O(n^{3/2})$ for 2-dimensional meshes, and $O(n^{5/3})$ for 3-dimensional meshes, where n is the number of meshpoints. The new algorithm is also practically faster by about a factor of four on a set of test problems.

We also varied the weights of the local and global terms in the priority function, and to our surprise, found that our test problems fell into two classes with different asymptotic behaviors of their wavefronts. When the first term is more important in reducing the wavefront, the problem belongs to Class 1, and when the second term is more important, it belongs to Class 2. We have observed that the first class of problems represent simpler meshes: e.g., discretization of the space surrounding a body, such as an airfoil. By choosing the weights of the two terms in priority function to suit each class of problems, we reduced the wavefront computed by the Sloan algorithm by about a third.

An algebraic algorithm

In joint work with Dr. Horst Simon and Dr. Stephen Barnard, I proposed a novel algebraic algorithm for the wavefront minimization problem. The algorithm associates a discrete Laplacian matrix with the given mesh, and then computes an

eigenvector corresponding to the smallest nonzero Laplacian eigenvalue. The ordering is obtained by sorting the components of this eigenvector in increasing or decreasing order.

The spectral algorithm can obtain significantly smaller wavefronts compared to the combinatorial algorithms for this problem. The success of this simple algorithm is somewhat intriguing. In recent work, Professor Alan George of Waterloo and I have provided stronger justification than was available for this algorithm.

We begin by considering the related problem of minimizing the 2-sum of a graph. Given an ordering of the vertices of a graph (from 1 to n , the number of vertices), compute the square of the difference in the numbers assigned to the endpoints of each edge, and then sum this quantity over all edges to obtain the 2-sum. The problem is that of computing the minimum 2-sum over all orderings of the graph.

We can formulate the 2-sum problem as a quadratic assignment problem (QAP) of the form

$$\min_{X \text{ permutation matrix}} \text{trace } QXBX^T,$$

where Q is the Laplacian matrix. B is the rank-one matrix with $b_{ij} = ij$, and the minimization is over the set of permutation matrices X . Unfortunately, this problem is NP-complete, and hence it is unlikely that there is a polynomial time algorithm for this problem.

We can make progress by minimizing over a larger set than the permutation matrices. We relax the requirement that X have nonnegative elements, while preserving the properties of X being orthogonal and having row and column sums equal to one. This leads to a lower bound for the 2-sum problem by means of a projection technique. We can show that the permutation matrix closest to the orthogonal matrix that attains the lower bound is obtained by permuting the second Laplacian eigenvector in increasing or decreasing order. This provides a *raison d'être* for the spectral algorithm.

It is also somewhat surprising that the lower bounds obtained are quite tight (within a factor of two) for the unstructured meshes that we have tested. These lower bounds show that the spectral reordering algorithm can yield nearly optimal values of the 2-sum, in spite of the fact that minimizing the 2-sum is an NP-complete problem. To

the best of our knowledge, these are the first results providing reasonable bounds on the quality of the orderings generated by a reordering algorithm for minimizing envelope-related parameters. Earlier work had not addressed the issue of the quality of the orderings generated by the algorithms. We have also shown that problems with bounded separator sizes (n^γ) have bounded wavefronts ($n^{1+\gamma}$).

Our analysis further shows that the spectral orderings attempt to minimize the 2-sum rather than the wavefront. Hence a reordering algorithm could be used in a post-processing step to improve the envelope and wavefront parameters from a spectral ordering. Gary Kumfert and I have used the Sloan algorithm to refine the ordering produced by the spectral algorithm to further reduce the wavefront. Currently this algorithm computes the lowest values of the wavefront on a collection of finite element meshes.

Conclusions

Gary Kumfert and I have designed object-oriented software in C++ for the Sloan, RCM, and the hybrid algorithms. It is available with three interfaces: PETSc (Argonne National Labs.), MATLAB, and as stand-alone code.

Current work involves extending the Sloan algorithm for anisotropic problems by considering an edge-weighted version. We are also investigating the application of another problem, the 1-sum problem, to the wavefront minimization problem. We are also continuing with more detailed formulations of the cache miss reduction problem.

References

- Stephen T. Barnard (Cray Research), Alex Pothén, and Horst D. Simon (Lawrence Berkely Lab), "A Spectral Algorithm for Envelope Reduction of Sparse Matrices," *Numerical Linear Algebra with Applications*, 2, pp. 317-334, 1995. (A shorter version appeared in Supercomputing '93.)
- Alan George (Waterloo) and Alex Pothén, "An Analysis of Spectral Envelope-Reduction via Quadratic Assignment Problems," *SIAM J. Matrix Analysis and its Applications*, 18, pp. 706-732, 1997.
- Gary K. Kumfert (ODU) and Alex Pothén, "Two Improved Algorithms for Reducing the Envelope Size and Wavefront of Sparse Matrices," *BIT*, 18 (3), pp. 559-590, 1997.

ICASE Colloquia

October 1, 1997 – December 31, 1997

- Hubona, Geoffrey S., Virginia Commonwealth University, "The Effects of Stereoscopic Viewing, Motion, and Object Shadows on Three-Dimensional Visualization," October 3.
- Interrante, Victoria, ICASE, "Strategies for Effectively Visualizing 3D Flow with Volume Line Integral Convolution," October 17.
- Loncaric, Josip, ICASE, "Sensor/Actuator Placement via Optimal Distributed Control of Exterior Stokes Flow," October 24.
- Povitsky, Alexander, ICASE, "Behavior of Vortical Density Inhomogeneity after Interaction with Shock and Expansion Waves," November 12.
- Chen, Po-Shu, University of Colorado at Boulder, "A Unified Framework of FETI Solver and its Applications," November 17.
- de Souza, Fenella, National Research Council, Canada, "On the Large Scale Organization of a Turbulent Boundary Layer Disturbed by a Circular Cylinder," December 15.

ICASE Reports

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- Alexandrov, Natalia, J.E. Dennis, Jr., Robert Michael Lewis, and Virginia Torczon: *A trust region framework for managing the use of approximation models in optimization*. ICASE Report No. 97-50, (NASA CR-201745), October 2, 1997, 19 pages. Submitted to Structural Optimization.
- Guattery, Stephen, Tom Leighton, and Gary L. Miller: *The path resistance method for bounding the smallest nontrivial Eigenvalue of a Laplacian*. ICASE Report No. 97-51, (NASA CR-201746), October 6, 1997, 20 pages. Submitted to Combinatorics, Probability, and Computing.
- Hesthaven, J.S., and L.M. Jameson: *A wavelet optimized adaptive multi-domain method*. ICASE Report No. 97-52, (NASA CR-201747), October 8, 1997, 21 pages. Submitted to Journal of Computational Physics.
- Ristorcelli, J.R., and G.A. Blaisdell: *Validation of a pseudo-sound theory for the pressure-dilatation in DNS of compressible turbulence*. ICASE Report No. 97-53, (NASA CR-201748), October 16, 1997, 14 pages. To appear in the Proceedings of the 11th Turbulent Shear Flow Symposium, Grenoble, France.

Girimaji, Sharath S.: *Dynamical system analysis of Reynolds stress closure equations*. ICASE Report No. 97-54, (NASA CR-201749), October 17, 1997, 17 pages. To appear in the Proceedings of the 11th Turbulent Shear Flow Symposium, Grenoble, France.

Allan, Brian G., Maurice Holt, and Andrew Packard: *Simulation of a controlled airfoil with jets*. ICASE Report No. 97-55, (NASA CR-201750), October 16, 1997, 21 pages. To appear in the Journal of Guidance, Control, and Dynamics.

Banerjee, Nana S., and James F. Geer: *Exponential approximations using Fourier series partial sums*. ICASE Report No. 97-56, (NASA CR-201751), October 20, 1997, 42 pages. Submitted to SIAM Journal on Scientific Computation.

Arian, Eyal: *Convergence estimates for multidisciplinary analysis and optimization*. ICASE Report No. 97-57, (NASA CR-201752), October 17, 1997, 39 pages. To appear in Progress in Systems and Control Theory (Birkhäuser Volume).

Girimaji, S.S., and J.R. Ristorcelli: *On the behavior of velocity fluctuations in rapidly rotating flows*. ICASE Report No. 97-58, (NASA CR-97-206244), November 17, 1997, 21 pages. To be submitted to Journal of Fluid Mechanics.

del Rosario, R.C.H., and R.C. Smith: *LQR control of thin shell dynamics: Formulation and numerical implementation*. ICASE Report No. 97-59, (NASA CR-97-206245), November 13, 1997, 33 pages. Submitted to Journal of Intelligent Material Systems and Structures.

Calkins, F.T., R.C. Smith, and A.B. Flatau: *An energy-based hysteresis model for magnetostrictive transducers*. ICASE Report No. 97-60, (NASA CR-97-206246), November 17, 1997, 21 pages. Submitted to IEEE Transactions on Magnetics.

Lewis, Robert Michael: *Numerical computation of sensitivities and the adjoint approach*. ICASE Report No. 97-61, (NASA CR-97-206247), November 17, 1997, 19 pages. Submitted to the Proceedings of the AFOSR Workshop on Optimal Design, Arlington, VA (Sept. 30 - Oct. 3, 1997).

Bataille, F., Ye Zhou, and Jean-Pierre Bertoglio: *Energy transfer and triadic interactions in compressible turbulence*. ICASE Report No. 97-62, (NASA CR-97-206249), November 19, 1997, 30 pages. To be submitted to Journal of Fluid Mechanics.

Rubinstein, Robert, and Ye Zhou: *The dissipation rate transport equation and subgrid-scale models in rotating turbulence*. ICASE Report No. 97-63, (NASA CR-97-206250), November 19, 1997, 17 pages. To appear in Proceedings of the 11th Turbulent Shear Flow Conference.

Yeung, P.K., and Ye Zhou: *On the universality of the Kolmogorov constant in numerical simulations of turbulence*. ICASE Report No. 97-64, (NASA CR-97-206251), November 21, 1997, 18 pages. Submitted to Physical Review E.

Shu, Chi-Wang: *Essentially non-oscillatory and weighted essentially non-oscillatory schemes for hyperbolic conservation laws*. ICASE Report No. 97-65, (NASA CR-97-206253), November 21, 1997, 83 pages. To appear in Lecture Notes in Mathematics, CIME Subseries, Springer Verlag.

Buchholz, Peter, Gianfranco Ciardo, Susanna Donatelli, and Peter Kemper: *Complexity of Kronecker operations of sparse matrices with applications to the solution of Markov models*. ICASE Report No. 97-66, (NASA CR-97-206274), December 18, 1997, 29 pages. To be submitted to INFORMS Journal on Computing.

Ciardo, Gianfranco, and Marco Tilgner: *Parametric state space structuring*. ICASE Report No. 97-67, (NASA CR-97-206267), December 10, 1997, 30 pages. Submitted to IEEE Transactions on Software Engineering.

Jameson, Antony: *Essential elements of computational algorithms for aerodynamic analysis and design*. ICASE Report No. 97-68, (NASA CR-97-206268), December 10, 1997, 71 pages.

Arian, Eyal, and Manuel D. Salas: *Admitting the inadmissible: Adjoint formulation for incomplete cost functionals in aerodynamic optimization*. ICASE Report No. 97-69, (NASA CR-97-206269), December 10, 1997, 18 pages. To be submitted to AIAA Journal.

Chieh, Tzi-Cker, and Kwan-Liu Ma: *A parallel pipelined renderer for time-varying volume data*. ICASE Report No. 97-70, (NASA CR-97-206275), December 18, 1997, 17 pages. Submitted to the International Journal in High Performance Computer Graphics, Multimedia and Visualisation.

Soemarwoto, Bambang: *The variational method for aerodynamic optimization using the Navier-Stokes equations*. ICASE Report No. 97-71, (NASA CR-97-206277), December 19, 1997, 32 pages. To be submitted to Computer and Fluids.

Hayder, M. Ehtesham, David E. Keyes, and Piyush Mehrotra: *A comparison of PETSC library and HPF implementation of an archetypal PDE computation*. ICASE Report No. 97-72, (NASA CR-97-206278), December 19, 1997, 27 pages. Submitted to Journal for Advances in Engineering Software.

Keyes, David E., Dinesh K. Kaushik, and Barry F. Smith: *Prospects for CFD on petaflops systems*. ICASE Report No. 97-73, (NASA CR-97-206279), December 19, 1997, 30 pages. Submitted to CFD Review 1997.

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